

## REMARKS

Applicants' claim of priority is noted but rejected in Paragraph 2 of the Office Action.

Applicants respectfully traverse certain of the assertions of Paragraph 2 and request further clarification, as set forth below. The Examiner's assertions are addressed individually.

- A. "[P]rovisional Application No. 60/235,336 does not support or enable the steps of providing samples spectra and measurements of a predetermined characteristic associated with the sample spectra."

In the "Nonlinear Optimization of Filter Layers" section, the provisional application refers to use of "a calibration set of optical spectra(s) representative of real samples," where the "concentration values (y) of the samples" is known. That is, the provisional application describes the provision of sample spectra (the optical spectra(s) representative of real samples) and measurements of a predetermined characteristic (the known concentration values (y) of the samples) associated with the sample spectra.

- B. "[P]rovisional Application No. 60/235,336 does not support or enable the steps of . . . selecting an initial number of layers [and] selecting a thickness for each layer."

In the "Nonlinear Optimization of Filter Layers" section, above equation 16, the provisional application describes initialization of the algorithm "by a specified number of layers (n) with either random or pre-determined thicknesses (z)."

- C. "[P]rovisional Application No. 60/235,336 does not support or enable the steps of . . . defining a first regression formula that relates interaction of light with the transmission spectra to a regression value."

In the "Nonlinear Optimization of Filter Layers" section, the provisional application describes a first regression formula with respect to equations 13 and 14. As described in the text, the formula relates an interaction of light (optical spectras) with the transmission spectrum (T) to a regression value ( $y_{\text{hat}}$ ).

- D. “[P]rovisional Application No. 60/235,336 does not support or enable the steps of . . . applying each sample spectrum to the regression formula, thereby determining the regression value for each sample spectrum.”

In the “Nonlinear Optimization of Filter Layers” section, the provisional application explains that “the vector of concentration ( $y_{\text{hat}}$ ) values of all the samples is predicted” by application of equation 14.

- E. “[P]rovisional Application No. 60/235,336 does not support or enable the steps of . . . defining a comparison relationship between the regression values and said measurements.”

In the “Nonlinear Optimization of Filter Layers” section, the provisional application describes SEP equation 15 that defines a comparison relationship between the regression values ( $y_{\text{hat}}$ ) and the measurement values ( $y$ ) of the samples.

- F. “[P]rovisional Application No. 60/235,336 does not support or enable the steps of. . . optimizing the comparison relationship for said regression values, wherein thickness of each said layer is an optimization variable.”

In the “Nonlinear Optimization of Filter Layers” section, in the text following equation 15, the provisional application describes the optimization of SEP equation 15, including layer thickness as an optimization variable.

- G. “[P]rovisional Application No. 60/235,336 does not support or enable the steps of. . . selecting a plurality of sets of initial conditions [and] selecting a group of layer thicknesses.”

In the “Nonlinear Optimization of Filter Layers” section, in the text following equation 20, the provisional application describes two variants to the filter design algorithm. In the first, the process begins with different random starts, each initialized with a specified number of layers with random thicknesses. Thus, the “search direction proceeds to different local minima on the response surface[,] hence the possibility of different solutions to the optimization problem.”

- H. [P]rovisional Application No. 60/235,336 does not support or enable the steps of . . . determining a second regression formula.”

In the “Nonlinear Optimization of Filter Layers” section, following equation 20, the provisional application describes a second variant to the filter design algorithm, in which the initial starting point is defined by first minimizing the sum of squared differences between a p-factor PCR regression vector and the calculated regression vector described above.

- I. “[P]rovisional Application No. 60/235,336 does not support or enable the steps of . . . actually forming an optical filter segment in the manner required by claims 11-19, 23, and 24.”

The provisional application does not describe methods of forming optical filters including all the limitations of any claims 11, 12, 23 and 24.

Furthermore, Applicants note that the two Soyemi, et al. articles form the basis for all claim rejections under 35 USC Sections 102 and 103, as set forth in paragraphs 17, 21 and 23 of the Office Action. The Soyemi articles, and particularly the Proceeding of SPIE, Vol. 4205 (2001) article (Soyemi 1), have disclosures similar in scope to the provisional application, with respect to the design algorithm. Thus, Applicants respectfully request clarification regarding what elements of claims 1-10 and 20-22 are not enabled by Provisional Application 60/235,336 but are sufficiently described by an enabling disclosure in either of the Soyemi articles so as to support a rejection under Sections 102 or 103.

Applicants also submit, however, that the material relied upon in the Soyemi articles is not properly the basis of the prior art rejections in that it represents Applicants’ own work. The three inventors of the present application, Myrick, Soyemi and Gemperline, are joint authors of both articles. Of the remaining authors, Zhang, Eastwood, Li, and Karunamuni

were graduate and post doctoral assistants working under the direction of one of the inventors and were not inventors of the subject matter of the claims of the present application.

Similarly, Mr. Synowicki provided test data at the request of one of the inventors and was not an inventor of the subject matter of the present claims.

More specifically, and as set forth in the affidavit of Dr. Michael L. Myrick attached hereto at E, the non-inventor joint authors performed experimental or testing work at Dr. Michael L. Myrick's direction. Eastwood and Zhang acquired sample spectra that were applied to a design algorithm and that is reflected in Figure 3 at page 1072 of Soyemi 2. Li recorded the data represented at Fig. 4C at page 1073 of Soyemi 2. Karunamuni was responsible for construction and maintenance of a deposition chamber in which optical filters were formed as described in Soyemi 2. Mr. Synowicki was employed by an entity that was independent of the inventors. Dr. Myrick sent samples of Nb<sub>2</sub>O<sub>5</sub> and SiO<sub>2</sub> to Mr. Synowicki, who performed a variable-angle spectroscopic ellipsometry analysis for the samples and provided resulting data to Dr. Myrick, as reflected in Fig. 2 at page 1071 of Soyemi 2.

With regard to Soyemi 1, Eastwood and Zhang acquired sample spectral data reflected in Fig. 4 at page 295. The data acquired by Li and reflected in Fig. 4C of Soyemi 2 was used in conjunction with the data reflected in Fig. 4 of Soyemi 1 to develop the information in Fig. 5 of Soyemi 1.

Accordingly, Applicants respectfully request that the rejections based on the Soyemi articles, as set forth in paragraphs 17, 21 and 23 of the Office Action, be removed.

Claims 2, 3, 16, and 24 were rejected under 35 USC Section 112 as set forth in paragraphs 8-12 of the Office Action. Applicants respectfully traverse these rejections.

Claims 2 and 3 were rejected on the grounds that it is unclear how light can be transmitted or reflected “by said transmission spectrum.” As noted in the present specification, for example in the Background of the Invention section at page 17, lines 1-6, a filter’s transmission spectrum is, collectively, the transmission percentages defined by the filter over its wavelength range. For example, if the filter’s transmission spectrum has a transmittance of 60% at a given wavelength, 60% of incident light at that wavelength is transmitted by the filter, and 40% is reflected. As indicated at page 17, a regression formula may include the difference between the filter’s transmitted and reflected light – i.e. the light transmitted by the transmission spectrum and the light reflected by the transmission spectrum.

Accordingly, Applicants submit that claims 2 and 3 are not indefinite as originally filed. To facilitate prosecution of the present application, however, Applicants have amended claim 2 to refer to light transmitted and reflected according to the transmission spectrum.

Claim 3 was rejected as indefinite, as set forth in paragraph 9 of the Office Action, in that the reference to “the spectrum of said light” is unclear. Applicants respectfully traverse this rejection. As the phrase at issue is “the spectrum of said light,” it is clear that the spectrum is that of “said light,” not the “sample spectrum” or the “transmission spectrum.” Claim 1 provides antecedent basis for “said light,” and since light inherently has a spectrum, use of “the” before “spectrum” is appropriate. Thus, there should be no confusion among “transmission spectrum,” “sample spectrum” and “the spectrum of said light.”

Claim 16 was rejected, as set forth in paragraph 10, as ambiguous regarding recitation of step (o). Claim 16 has been amended to correct a typographical error, replacing (o) with (n). Applicants submit that the rejection has thereby been overcome.

Claims 20 – 24 have been rejected, as set forth in paragraph 11, regarding recitation of optimizing said comparison relationship for said regression values to a minimum said “regression value.” Applicants submit that the claim recitation is not indefinite, in that the cited phrase refers to optimizing the comparison relationship until the comparison value reaches a minimum level. To facilitate prosecution of the present application, however, claims 1, 20 and 24 have been amended to clarify that the comparison relationship is optimized for regression values based on minimization of, or defines a comparison value based on, differences between the regression values and the measurements. Claims 1 and 20 have been amended to clarify that the comparison relationship compares the regression values and the measurements.

Claim 23 has been rejected as set forth in paragraph 12 of Office Action. Claim 23 has been amended to overcome the rejection.

Claim 3 has been amended to clarify antecedent basis for “spectrum” in line 3.

Claim 10 has been amended to correct a typographical error.

Claims 11, 12, 19, 23 and 24 have been amended to clarify antecedent basis of “optical interference filter.”

Claim 13 has been amended to clarify antecedent basis regarding “first layer.”

Claim 14 has been amended to clarify antecedent basis of “difference” in view of the amendments to claim 1.

Claims 16 and 19 have been amended to clarify the identification of the layer from the previous step (i).

Claim 23 has been amended to clarify antecedent basis regarding “thickness.”

Claim 24 has been amended to clarify the identification of the layer from the previous step (k).

The specification has been amended to correct references to an equation.

Claims 1 through 24 were rejected under 35 USC Section 112, first paragraph, as set forth in paragraph 14 of the Office Action. In general, the claims were rejected on the grounds that the specification fails to enable one skilled in the art to practice the invention commensurate in scope with the claims without undue experimentation, in that certain elements of the claims are broader in scope than examples expressly described in the specification.

Applicants respectfully traverse the rejection. The subject matter of the present claims are in the predictable arts, and where claims in such arts are broader in scope than specific examples that may be expressly provided in the specification, those of ordinary skill in the relevant art can generally understand, in view of the specification, that the specification may support a broader subject matter. The Office Action does not point to any implication in the present application that the invention is limited to expressly disclosed embodiments or otherwise to subject matter narrower than the scope of the claims. Instead, the Office Action takes the position that the claims are not enabled merely if they encompass a scope broader than the expressly disclosed embodiments. Applicants therefore submit that the rejection is improper.

In any event, Applicants respectfully submit that one skilled in the art, in view of the disclosure of the present specification, would recognize that the specification enables the full scope of the claims. Taking the points raised in the Office Action in turn:

- A. The claims are open to any “sample spectra” and any “predetermined characteristic measurements, but the Applicants’ disclosure is limited to sample spectra of gasoline samples and octane value measurements;

The claims of the present application are directed to methods of determining layer thicknesses for optical interference filters. The methods begin with the step of providing sample spectra and measurements of a predetermined characteristic associated with respective sample spectra, but those skilled in the art should recognize, in view of the present specification, that gasoline octane value is merely an example and that the particular sample and associated characteristic can vary with the user's needs. As indicated in U.S. Patent 6,198,531 (the disclosure of which is incorporated by reference in the specification of the present application), light samples can carry a variety of information, for example ethylene content of polymer samples, blood glucose level and information for long range optical communications in wavelength-division multiplexing systems. Further, Applicants attach at A an image of a front cover of the March, 2000 issue of Applied Spectroscopy, which reflects the known chemometric procedure of acquiring samples, performing lab analysis on the samples to determine desired characteristics and spectra of the samples, and modeling the spectra to establish how the spectra are related to the characteristics. One skilled in the art would not view the disclosure in the present specification regarding sample spectra and predetermined characteristics associated with the sample spectra as limited to gasoline octane rating but rather would understand that the claimed method could be applied to a variety of subject samples as desired.



- B. The claims are open to any method of “determining a transmission spectrum,” but the Applicants’ disclosure is limited to using a specific matrix method to determine the transmission spectrum;

It is known in the art how to determine a transmission spectrum of an optical filter once the number of layers and the thickness and composition of the layers are known. Exemplary steps for such a procedure are described as prior art in the Background section of the present application, beginning at page 5, line 5, and it is also noted in the Background section that commercially available software (TFCALC, available from Software Spectra, Inc.) can perform this function. Pages 44-49 of the Handbook of Infrared Spectroscopy of Ultrathin Films (2003), a copy of which is attached hereto at B, describe recursive and matrix methods of determining transmission spectra. Applicants respectfully submit that one skilled in the art, in view of the present specification, would understand the specification is not limited to any particular method expressly described in the specification of determining transmission spectra and that the specification enables the full scope of the claims with respect to determining a transmission spectrum of an optical filter having a selected number of layers and a selected thickness of each layer.

- C. The claims are open to any method of “defining” a regression formula, but the Applicants’ disclosure is limited to using a specific method to define a specific regression formula.

Regression analysis is a well known and understood statistical tool, as reflected in the March, 2000 Cover of Applied Spectroscopy attached at A and the following definitions from McGraw-Hill Dictionary of Scientific and Technical Terms, 1679 (5<sup>th</sup> ed., 1993) (Attachment C):

Regression - “given two stochastically dependent random variables, regression functions measure the mean expectation of one relative to the other.”

Regression Analysis - “the description of the nature of the relationship between two or more variables; it is concerned with the problem of describing or estimating the value of the dependent variable on the basis of one or more independent variables.

Regression Coefficient – “the coefficient of the independent variables in a regression equation.”

Regression Estimate – “an estimate of one variable obtained by substituting the known value of another variable in a regression equation calculated on sample values of the two variables.”

Applicants respectfully submit that one skilled in the art, upon reading the present specification, would understand that the specification is not limited to any particular method expressly described in the specification for defining regression formulas and that the specification enables the full scope of the claims with respect to defining a regression formula.

- D. The claims are open to any method of “defining a comparison relationship” between regression values and measurements, [but] the Applicants’ disclosure is limited to doing so by using a specific merit function; and
- E. The claims are open to any method of “optimizing said comparison relationship” for the regression values, but the Applicants’ disclosure is limited to doing so by a specific method.

Referring to the defining and optimizing steps together, Applicants note that the optimization of comparison relationships among multiple variables is a well known and understood mathematical process. For example, the Background section of the present application describes a prior art method of designing an optical filter beginning with a desired transmission spectrum and a selection of materials for the filter layers. A merit function describes the difference between the desired spectrum and any other spectrum. Given a

starting point for the number of filter layers and thicknesses thereof in the “other” spectrum, the values for the number of filter layers and layer thicknesses are varied in order to optimize the merit function value and thereby identify an “other” spectrum closest to the desired spectrum based on the original starting point. A quasi-Newton method of optimization is described. It is also noted in the Background section that commercially available software (TFCALC, available from Software Spectra, Inc.) can perform these functions.

As indicated in the Background section, one skilled in the art should understand that various comparison relationships may be defined, for example as described at equations 1a, 1b and 1c. Moreover, once the comparison relationship is defined, one skilled in the art should recognize that an optimization method other than a quasi-Newton method could be employed. For instance, the description of a “quasi” Newton method should indicate that a Newton method could be used. Newton’s method is a basic mathematical process, defined at McGraw-Hill Dictionary of Scientific and Technical Terms, 1081 (3<sup>rd</sup> ed., 1983) (Attachment D) as “a technique to approximate the roots of an equation by the methods of the calculus.”

As noted in the Office Action, prior art patents recognize that it is known to minimize merit function values in designing optical filters. At col. 10, lines 28-52, US Patent 4,896,928 describes a method of designing an optical filter based on a desired reflectance spectrum:

Those of ordinary skill in the art will be familiar with, and capable of performing such an iterative optimization operation, as a matter of routine design. The operation will typically [include]

the steps of choosing a merit function, and then minimizing the merit function utilizing an optimization routine, to determine the optimal set of design parameters. For example, U.S. Pat. No. 4,536,063, issued Aug. 20, 1985 to Southwell . . . , discusses the manner in which an optical coating design merit function may be chosen, and then minimized, to generate a desired optical coating design.

Applicants respectfully submit that one skilled in the art, upon reading the present specification, would understand that the specification is not limited to any specific method expressly described in the specification for defining a comparison relationship between regression values and sample spectra measurements or of optimizing the relationship and that the specification enables the full scope of the claims as originally filed with respect thereto.

For at least these reasons, Applicants traverse the rejection of claims 1-24 under 35 USC § 112, first paragraph, for lack of enablement.

Applicants submit that the application is in condition for allowance. Favorable action, and withdrawal of outstanding rejections, is therefore respectfully requested. The Examiner is requested to contact the undersigned at his convenience should any issues remain.

Respectfully submitted,

NELSON MULLINS RILEY  
& SCARBOROUGH, L.L.P.

A handwritten signature in black ink, appearing to read 'Lloyd G. Farr', is written over a horizontal line.

Lloyd G. Farr  
Registration No. 38,446

1320 Main Street  
Columbia, SC 29201  
(404) 817-6165  
Fax (803) 255-9831

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# HANDBOOK OF INFRARED SPECTROSCOPY OF ULTRATHIN FILMS

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Valeri P. Tolstoy  
Irina V. Chernyshova  
Valeri A. Skryshevsky

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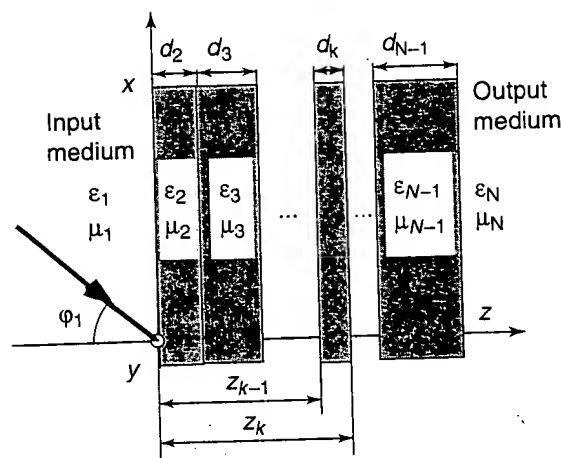
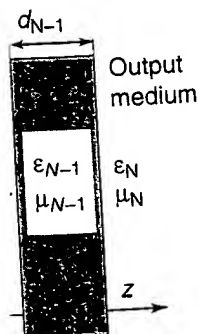


Figure 1.14. Scheme of stratified medium containing  $N$  phases and  $N - 2$  layers. Shown are coordinates and nomenclature used throughout.

and the matrix method — both requiring computer programming. In the limiting cases, these approaches permit one to study wave propagation phenomena for a transition (inhomogeneous in depth) layer by “slicing” it into a large enough number of infinitely thin layers and, for a single layer, by equating this number to unity. Abeles [129, 130] was the first to suggest the use of  $2 \times 2$  matrix transformations to simplify the calculations of the optical response in the case of isotropic layers. Abeles’s formalism was developed [9, 52, 87, 131, 132] into a more convenient form for computation by introducing the Fresnel coefficients. Harbecke [133] and Ohta and Ishida [134] extended Abeles’s approach to a system with phase incoherence, based on the concept of incoherent multiple reflections in real systems, in which there are neither plane nor parallel surfaces nor a monochromatic light source or some layers are sufficiently thick so that the period of interference is smaller than the resolution of the spectrometer.

The mathematical treatment of light propagation through an anisotropic stratified medium is not simple. Exact solutions can be obtained by the  $4 \times 4$  matrix method [14, 135–139] generalizing Abeles’s approach to anisotropic layers. The advantage of the Berreman  $4 \times 4$  formalism [135] is in its applicability to materials with magnetic anisotropy and optically active materials. For the determination of orientation within the media, Parikh and Allara [138] found Yeh’s treatment of the  $4 \times 4$  matrix method [14] to be most flexible, extending it to a pile of absorbing films, each with any degree of anisotropy up to and including biaxial symmetry. However, according to Cojocaru [140], for practical purposes, the so-called  $2 \times 2$  extended Jones matrix method [131] is adequate and easier to use. Hasegawa et al. [141] demonstrated that Hansen’s  $2 \times 2$  matrix method can be easily generalized for the case of anisotropy by introducing Drude’s formulas developed originally for a two-anisotropic-phase system. They presented the matrix method for uniaxial media and tested it in the studies of the molecular



orientation (MO) in the multilayered Langmuir-Blodgett films with uniaxial symmetry. Yamamoto and Ishida [115, 142] extended Hansen's method to the case of biaxial anisotropy. Based on the matrix method of Ohta and Ishida [134] and the generalization of Yamamoto and Ishida [115, 142], Buffeteau et al. [143] suggested the computation procedure applicable for an arbitrary succession of coherent anisotropic and incoherent layers.

In this section, we shall give the recursion relationships derived by Popov [144] and Leng et al. [145] and the explicit formulas and algorithm for programming the spectral simulations according to the Hansen matrix method [100], applicable to isotropic thin films. For the most part, the spectral simulations in the present handbook were carried out by using the program based on this algorithm. In Chapters 2 and 3 we will show that, using such a program or recursion relationship, any spectroscopist can simulate the IR spectra for the layered system of interest. The simulated spectra provide extensive information, assisting in, for example, the determination of the optimum conditions for recording the spectrum (Chapter 2) and the interpretation of the spectrum (Chapter 3).

1.7.1°. Let there be a general system of  $N$  isotropic layers with different optical properties (described by the complex refractive indices  $\hat{n}_j$ ) and of arbitrary thicknesses  $d_j$  (Fig. 1.14). The recursion relationship of the corresponding reflectance that is conducive to computer programming has been obtained in [144]. In the case  $\varphi_1 = 0$ ,

$$R^{s,p} = \left| h_1 + \frac{h_2^2}{-h_1 + \frac{1}{h_3 + \frac{h_4^2}{-h_3 + \frac{1}{h_5 \cdots + \frac{h_{2j-2}^2}{-h_{2j-3} + 1/h_{2j-1}}}}} \right|^2 \quad (1.102)$$

with the intermediate variables defined as

$$h_{2j} = \frac{(1 - r_j^2)e^{-ik\hat{n}_j d_j}}{1 - r_j^2 e^{-2ik\hat{n}_j d_j}}, \quad (1.103)$$

$$h_{2j-1} = r_j \frac{1 - e^{-2ik\hat{n}_j d_j}}{1 - r_j^2 e^{-2ik\hat{n}_j d_j}},$$

$$r_j = -\frac{\hat{n}_j - 1}{\hat{n}_j + 1}, \quad (1.104)$$

where  $k = 2\pi/\lambda$  and  $\lambda$  is the wavelength in a vacuum. For  $\varphi_1 \neq 0$  and  $p$ -polarization,  $\hat{n}_j$  is replaced by  $\hat{n}_j \cos \varphi_j$  in Eq. (1.103) and by  $|\hat{n}_j| \cos \varphi_j$  in Eq. (1.104), whereas for  $s$ -polarization,  $\hat{n}_j$  is replaced by  $\hat{n}_j \cos \varphi_j$  in Eq. (1.103)

computer programming. In the limiting wave propagation phenomena for by "slicing" it into a large enough single layer, by equating this number to suggest the use of  $2 \times 2$  matrix of the optical response in the case developed [9, 52, 87, 131, 132] into introducing the Fresnel coefficients. extended Abeles's approach to the concept of incoherent multiple layers are sufficiently thick so that the resolution of the spectrometer. propagation through an anisotropic strat- can be obtained by the  $4 \times 4$  matrix. s approach to anisotropic layers. The [135] is in its applicability to materi- active materials. For the determination d Allara [138] found Yeh's treatment most flexible, extending it to a pile of anisotropy up to and including biax- caru [140], for practical purposes, the method [131] is adequate and easier to. at Hansen's  $2 \times 2$  matrix method can- isotropy by introducing Drude's formu- opic-phase system. They presented the- sted it in the studies of the molecular



and by  $(\cos \varphi_j)/\hat{n}_j$  in Eq. (1.104). The complex refractive index  $\hat{n}_j$  and the complex angle of incidence  $\varphi_j$  follow Snell's law (1.56). Equation 1.102 is seldom used for spectral simulations, perhaps being as of yet relatively unknown.

For analysis of six-layer silicon on oxide films, Leng et al. [145] applied the following elegant regression formula:

$$R_n^{s,p} = \left( \frac{r_n^{s,p} + R_{n+1}^{s,p}}{1 + r_n^{s,p} R_{n+1}^{s,p}} \right) e^{2ik_{n,z}d_n}, \quad (1.105)$$

where  $d_n$  is the thickness of the  $n$ th layer,  $R_n^{s,p}$  is the reflectance of the  $s$ - or  $p$ -polarized radiation from layer  $n$ , and  $r_n^{s,p}$  is the Fresnel coefficients for the interface between layers  $n$  and  $n+1$ , calculated as

$$r_n^s = \frac{\mu_{n+1}k_{n,z} - \mu_n k_{n+1,z}}{\mu_{n+1}k_{n,z} + \mu_n k_{n+1,z}}, \quad r_n^p = \frac{\hat{\epsilon}_{n+1}k_{n,z} - \hat{\epsilon}_n k_{n+1,z}}{\hat{\epsilon}_{n+1}k_{n,z} + \hat{\epsilon}_n k_{n+1,z}},$$

where  $\hat{\epsilon}_n$  and  $\mu_n$  are the permittivity and permeability of the material in layer  $n$ , respectively, and  $k_{n,z} = (2\pi/\lambda)(n_n + ik_n) \cos \varphi_n$  ( $\varphi_n$  is the angle of propagation in the  $n$ th layer). The Fresnel coefficients for each layer are calculated from the layer below.

**1.7.2°.** The theoretical background of the matrix method is covered in a great body of literature (see, e.g., Refs. [9, 14, 52, 87, 88, 131, 142]). The basic concept involves the construction of a characteristic transfer matrix for a pile of films,  $M$ , as the matrix product of the characteristic matrices of each film,  $M_j$ . In its turn, the characteristic matrix of a single film,  $M_j$ , is generated on the basis of the boundary conditions (1.4.7°). According to Abeles's approach [104, 105, 129, 130], such a matrix relates the tangential amplitudes of the electric and magnetic field vectors at the input and output film boundaries. The main characteristic matrix,  $M = \prod_j M_j$ , relates the tangential amplitudes of the electric and magnetic field vectors at the input,  $z = 0$ , and at the output boundary of the pile (Fig. 1.14). (The other type of matrix method uses amplitudes of the electric fields for directions of incidence and reflection [87, 132]. However, this method is not considered here since it cannot be generalized to anisotropy.) The Fresnel amplitude reflection and transmission coefficients of the system (1.4.5°) are expressed in terms of the matrix elements, which allows one to calculate the reflection and transmission spectra of the whole layered system.

**1.7.3°.** Let us now reproduce the algorithm of the Hansen method following the notations of Ref. [100]. The optical configuration used throughout the text is described in Fig. 1.14. Incoming parameters for the spectral simulations are as follows:

1. The number of media,  $N$ , of which 1st and  $N$ th are the medium of incidence and the final medium, respectively. The number of layers is, therefore,  $N - 2$ .

x refractive index  $\hat{n}_j$  and the complex extinction coefficient  $k(\nu)$  in the spectral range of interest. These dependences can (a) be calculated by using Eqs. (1.17) and (1.53) if the parameters of the corresponding oscillators are known, (b) be extracted from the reflection or absorption spectrum by the KK relations (1.18) (see description of the procedure, e.g., [142]), or (c) be reference data [16, 25, 47, 48, 51].

$$\left( \frac{1}{1} \right) e^{2ik_{n,z}d_n}, \quad (1.105)$$

$R_n^{s,p}$  is the reflectance of the s- or p-polarized light,  $F_n^{s,p}$  is the Fresnel coefficients for the interface between media  $n$  and  $n+1$  ated as

$$F_n^{s,p} = \frac{\hat{\epsilon}_{n+1}k_{n,z} - \hat{\epsilon}_n k_{n+1,z}}{\hat{\epsilon}_{n+1}k_{n,z} + \hat{\epsilon}_n k_{n+1,z}},$$

permeability of the material in layer  $n$ ,  $\varphi_n$  ( $\varphi_n$  is the angle of propagation) and  $\cos \varphi_n$  are calculated from the

the matrix method is covered in a. [14, 52, 87, 88, 131, 142]). The basic characteristic transfer matrix for a pile of characteristic matrices of each film,  $M_j$ . For a single film,  $M_j$ , is generated on the basis of the tangential amplitudes of the electric and magnetic fields at the input and output film boundaries. The main principle of the matrix method uses amplitudes of the electric and magnetic fields at the input and reflection [87, 132]. However, this method cannot be generalized to anisotropy. The transmission coefficients of the system (1.4.5) are calculated, which allows one to calculate the transmission coefficients of the whole layered system.

Algorithm of the Hansen method following the configuration used throughout the text is: The parameters for the spectral simulations are as

1st and  $N$ th are the medium of incidence. The number of layers is, therefore,

2. The wavenumber dependences of the real refractive index  $n(\nu)$  and the extinction coefficient  $k(\nu)$  in the spectral range of interest. These dependences can (a) be calculated by using Eqs. (1.17) and (1.53) if the parameters of the corresponding oscillators are known, (b) be extracted from the reflection or absorption spectrum by the KK relations (1.18) (see description of the procedure, e.g., [142]), or (c) be reference data [16, 25, 47, 48, 51].
3. The magnetic permeability  $\mu_j$  ( $j = 1, 2, \dots, N$ ) for each of the  $N$  media (1.1.2°).
4. The angle of incidence  $\varphi_1$ .
5. The thickness  $d_j$  for each of the  $N - 2$  layers.
6. The wavenumber range and step.

1.7.4°. The spectral simulation involves the stepwise calculation of the following quantities at each wavenumber, with the selected step over the range covered:

1. The complex vectors  $\hat{n}_j = n_j + ik_j$  and  $\hat{\epsilon}_j = n_j^2 - k_j^2 + 2in_jk_j$  ( $j = 1, \dots, N$ ).
2. The cosines of the complex angle of refraction,  $\cos \varphi_j = [1 - ((n_1 \sin \varphi_1)^2 / \hat{n}_j^2)]^{1/2}$ , as  $\cos \varphi_j = |\operatorname{Re}(\cos \varphi_j)| + i|\operatorname{Im}(\cos \varphi_j)|$ ,  $j = 2, \dots, N$ .
3. The generalized complex indices of refraction  $\xi_j \equiv \hat{n}_j \cos \varphi_j$  ( $j = 1, \dots, N$ ), Eq. (1.69), where  $\hat{n}_j$  is obtained at step 1 and  $\cos \varphi_j$  is found at step 2.
4.  $\beta_j \equiv 2\pi d_j \xi_j \nu_j$  ( $j = 1, \dots, N$ ), where  $\xi_j$  is the complex quantity obtained at step 3.
5.  $p_j = (\hat{\epsilon}_j / \mu_j)^{1/2} \cos \varphi_j$ .
6.  $q_j = (\mu_j / \hat{\epsilon}_j)^{1/2} \cos \varphi_j$ .
7. The elementary characteristic matrix  $M_j$  for each of the  $N - 2$  constituent layers in the particular stratified medium is calculated as

$$(a) M_j^s = \begin{vmatrix} \cos \beta_j & \frac{-i}{p_j} \sin \beta_j \\ -ip_j \sin \beta_j & \cos \beta_j \end{vmatrix} \quad \text{for } s\text{-polarization,}$$

$$(b) M_j^p = \begin{vmatrix} \cos \beta_j & \frac{-i}{q_j} \sin \beta_j \\ -iq_j \sin \beta_j & \cos \beta_j \end{vmatrix} \quad \text{for } p\text{-polarization.}$$

Here,  $i = \sqrt{-1}$  and  $j = 2, 3, \dots, N - 1$ .

8. The characteristic matrix of the whole multilayer structure is calculated as the product of the elementary matrices obtained at step 7:

$$M = M_2 M_3 \cdots M_{N-1} \equiv \begin{bmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{bmatrix}.$$

9. By using the elements of the  $M$  matrix, the Fresnel amplitude reflection and transmission coefficients (1.58) of the  $N$ -isotropic-phase medium are found from

$$\begin{aligned} r^s &= \frac{(m_{11} + m_{12}p_N)p_1 - (m_{21} + m_{22}p_N)}{(m_{11} + m_{12}p_N)p_1 + (m_{21} + m_{22}p_N)}, \\ r^p &= \frac{(m_{11} + m_{12}q_N)q_1 - (m_{21} + m_{22}q_N)}{(m_{11} + m_{12}q_N)q_1 + (m_{21} + m_{22}q_N)}, \\ t^s &= \frac{2p_1}{(m_{11} + m_{12}p_N)p_1 + (m_{21} + m_{22}p_N)}, \\ t^p &= \frac{2q_1}{(m_{11} + m_{12}q_N)q_1 + (m_{21} + m_{22}q_N)}. \end{aligned}$$

10. With the quantities computed at step 9, the reflectance and transmittance of the stratified medium are calculated as

$$\begin{aligned} \text{(a)} \quad R^{s,p} &= r^{s,p} \cdot r^{s,p*} = |r^{s,p}|^2, \\ \text{(b)} \quad T^s &= \frac{\mu_1 \operatorname{Re}(\hat{n}_N \cos \varphi_N)}{\mu_N n_1 \cos \varphi_1} |t^s|^2, \\ \text{(c)} \quad T^p &= \frac{\mu_N \operatorname{Re}(\hat{n}_N \cos \varphi_N / \hat{n}_N^2)}{\mu_1 n_1 \cos \varphi_1 / n_1^2} |t^p|^2. \end{aligned}$$

1.7.5°. Formulas may be derived on the basis of the matrix method for the reflectance and transmittance for a layer whose optical constants vary with the depth [9, 14, 87, 88, 109, 132, 146, 147]. For example, the following expressions for reflectance and transmittance were obtained in [147]:

$$R = \left| \frac{\sqrt{\zeta^2 + \chi^2}(r_{\text{sub}} + r_{f0}) + [\zeta(r_{\text{sub}} - r_{f0}) + \chi(1 + r_{\text{sub}}r_{f0})] \tanh(\sqrt{\zeta^2 + \chi^2})}{\sqrt{\zeta^2 + \chi^2}(1 + r_{\text{sub}}r_{f0}) + [\zeta(1 - r_{\text{sub}}r_{f0}) + \chi(r_{\text{sub}} + r_{f0})]} \right|^2, \quad (1.106)$$

$$T = \left| \frac{-\int_0^d \partial \hat{n}_f(z) / \partial z \cdot \hat{n}_f(z) / 2 [\hat{n}_f^2(z) - \hat{n}_{f0}^2 \sin \varphi_1]}{\cosh(\sqrt{\zeta^2 + \chi^2})(1 + r_{\text{sub}}r_{f0}) + \sinh(\sqrt{\zeta^2 + \chi^2}) \times [\chi(1 - r_{\text{sub}}r_{f0}) + \zeta(r_{\text{sub}} + r_{f0})]} \right|^2, \quad (1.107)$$

where  $r_{\text{sub}}$  is the Fresnel amplitude coefficient for the interface between the inhomogeneous film and the substrate,  $r_{f0}$  is the Fresnel amplitude coefficient for the interface between the surroundings and the film,  $\hat{n}_f(z)$  is the refractive index as a function of the film depth, and  $\hat{n}_{f0} = n_{f0} + ik_{f0}$  is the refractive

Fresnel amplitude reflection  
isotropic-phase medium are

$$\frac{r_{21} + m_{22}p_N}{r_{21} + m_{22}p_N},$$

$$\frac{r_{21} + m_{22}q_N}{r_{21} + m_{22}q_N},$$

$$\frac{r_{21} + m_{22}p_N}{r_{21} + m_{22}p_N},$$

$$\frac{r_{21} + m_{22}q_N}{r_{21} + m_{22}q_N}.$$

reflectance and transmittance

index of the film at the interface with the surroundings,

$$S_s = \int_0^d dz \frac{\partial \hat{n}_f(z)}{\hat{n}_f(z) \partial z} \left( 1 - \frac{\hat{n}_f^2(z)}{2[\hat{n}_f^2(z) - \hat{n}_{f0}^2 \sin \varphi_1]} \right),$$

$$S_p = \int_0^d dz \frac{\partial \hat{n}_f(z)}{\partial z} \left( \frac{\hat{n}_f(z)}{2[\hat{n}_f^2(z) - \hat{n}_{f0}^2 \sin \varphi_1]} \right),$$

$$\chi_s = \chi_p = \text{Im} \int_0^d dz \sqrt{\hat{n}_f^2 - \hat{n}_{f0}^2 \sin \varphi_1},$$

and  $\varphi_1$  is the angle of incidence.

1.7.6°. The Hansen formulas shown above can be adopted for anisotropic layers by redetermining the quantities  $\beta_j$ ,  $p_j$ , and  $q_j$ , introduced in (1.7.4°), in the following way [126, 142]:

- 4°.  $\beta_j^p \equiv 2\pi d_j v_j \hat{n}_{jx} \cos \varphi_j^p$ ,  $\beta_j^s \equiv 2\pi d_j v_j \hat{n}_{jy} \cos \varphi_j^s$  ( $j = 1, \dots, N$ , axes as shown in Fig. 1.14);
- 5°.  $p_j = \cos \varphi_{jp} / \hat{n}_{jx}$ ; and
- 6°.  $q_j = \hat{n}_{jy} \cos \varphi_{js}$ .

Here, the angles  $\varphi_{jp}$  and  $\varphi_{js}$  are defined by the equations  $\hat{n}_1 \sin \varphi_1 = \hat{n}_{jz} \sin \varphi_{jp}$  and  $\hat{n}_1 \sin \varphi_1 = \hat{n}_{jy} \sin \varphi_{js}$ , respectively, and  $\hat{n}_{jk} = n_{jk} + ik_{jk}$  ( $k = x, y, z$ ).

## 1.8. ENERGY ABSORPTION IN LAYERED MEDIA

According to Maxwell's theory, the rate at which radiation energy is absorbed is directly proportional to the *mean-square electric field* (MSEF),  $\langle E^2 \rangle$ , at the place where the absorption occurs (1.1.15°, 1.2.9°), which in turn is strongly dependent on the position within the layered medium, parameters of the experiment such as the polarization and the angle of incidence, and the material characteristics (the refractive indices of the layer, the substrate, and surroundings). Fry [148] proposed the use of the variation of the angle of incidence on the MSEF to determine optimal experimental conditions. This method, which is sometimes referred to as *electric field analysis* (EFA), has helped to understand the enhancement mechanisms in grazing-angle external reflection spectra of thin films on metals [101, 132, 149], *metal overlayer ATR* (MOATR) [2, 132, 150], and the ATR spectra of graphite-coated organic films [151]. Suzuki et al. [152] interpreted the phenomenon of spectral enhancement for ultrathin films on rough metal surfaces and islandlike metal underlayers using EFA. Sperline et al. [153, 154] proposed evaluation of surface excess of the adsorbed molecules at the solid-liquid interface in terms of the electric field intensities. Harbecke et al. [155] and Grosse and Offermann [2] interpreted the Berreman effect (Section 3.2) using the EFA expressions for the dissipated energy. By analyzing the electric field strengths,

is of the matrix method for the  
optical constants vary with the  
mple, the following expressions  
in [147]:

$$\left| \frac{r_{\text{sub}} - r_{f0}}{2 + \chi^2} \right|^2, \quad (1.106)$$

$$f_0) + \chi(r_{\text{sub}} + r_{f0})],$$

$$\left| \frac{\hat{n}_{f0}^2 \sin \varphi_1}{\sqrt{\chi^2 + \chi^2}} \right|^2, \quad (1.107)$$

$$f_0)]$$

at for the interface between the  
the Fresnel amplitude coefficient  
the film,  $\hat{n}_f(z)$  is the refractive  
 $f_0 = n_{f0} + ik_{f0}$  is the refractive

AB

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On the cover: Photomicrograph of crystals of vitamin B<sub>12</sub>.  
(Dennis Kunkel, University of Hawaii)

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**regmagenesis** [GEOL] Diastrophic production of regional strike-slip displacements. { 'reg-mə'jen-ə-səs }

**regmaglypt** [GEOL] Any of various small, well-defined, characteristic indentations or pits on the surface of meteorites, frequently resembling the imprints of fingertips in soft clay. Also known as pezoglyph; piezoglypt. { 'reg-mə,glip-t }

**regolith** [GEOL] The layer rock or blanket of unconsolidated rocky debris of any thickness that overlies bedrock and forms the surface of the land. Also known as mantle rock. { 'reg-ə,lith }

**Regosol** [GEOL] In early United States soil classification systems, one of an azonal group of soils that form from deep, unconsolidated deposits and have no definite genetic horizons. { 'reg-ə,säl }

**reggradation** [GEOL] The formation by a stream of a new profile of equilibrium, as when the former profile, after gradation, became deformed by crustal movements. { 'rē-grā'dā-shən }

**regression** [GEOL] The theory that some rivers have sources on the rainier sides of mountain ranges and gradually erode backward until the ranges are cut through. [OCEANOGR] Retreat of the sea from land areas, and the consequent evidence of such withdrawal. [PSYCH] A mental state and a mode of adjustment to difficult and unpleasant situations, characterized by behavior of a type that had been satisfying and appropriate at an earlier stage of development but which no longer befits the age and social status of the individual. [STAT] Given two stochastically dependent random variables, regression functions measure the mean expectation of one relative to the other. { ri'gresh-ən }

**regression analysis** [STAT] The description of the nature of the relationship between two or more variables; it is concerned with the problem of describing or estimating the value of the dependent variable on the basis of one or more independent variables. { ri'gresh-ən ə,nal-ə-səs }

**regression coefficient** [STAT] The coefficient of the independent variables in a regression equation. { ri'gresh-ən ,kō-ə,fish-ənt }

**regression conglomerate** [GEOL] A coarse sedimentary deposit formed during a retreat (recession) of the sea. { ri'gresh-ən kən,glām-ə-rət }

**regression curve** [STAT] A plot of a regression equation; for two variables, the independent variable is plotted as the abscissa and the dependent variable as the ordinate; for three variables, a solid model can be constructed or the representation can be reduced by an isometric chart or stereogram. { ri'gresh-ən ,kərv }

**regression estimate** [STAT] An estimate of one variable obtained by substituting the known value of another variable in a regression equation calculated on sample values of the two variables. { ri'gresh-ən ,es-tə-mət }

**regression line** [STAT] A linear regression equation with two or more variables. { ri'gresh-ən ,lin }

**regression of nodes** [ASTRON] The westward movement of the nodes of the moon's orbit; one cycle is completed in about 18.6 years. { ri'gresh-ən əv-'nōdz }

**regressive overlap** See overlap. { ri'gres-iv 'o-vər,lap }

**regressive reef** [GEOL] One of a series of nearshore reefs or bioherms superimposed on basinal deposits during the rising of a landmass or the lowering of the sea level, and developed more or less parallel to the shore. { ri'gres-iv 'rēf }

**regressive ripple** [GEOL] An asymmetric ripple mark formed by a current but oriented in a direction opposite to the general movement of current flow (steep side facing upcurrent). { ri'gres-iv 'rip-əl }

**regressive sediment** [GEOL] A sediment deposited during the retreat or withdrawal of water from a land area or during the emergence of the land, and characterized by an offlap arrangement. { ri'gres-iv 'sed-ə-mənt }

**regret criterion** See Savage principle. { ri'gret kri,tir-ē-ən }

**regula falsi** [MATH] A method of calculating an unknown quantity by first making an estimate and then using this and the properties of the unknown to obtain it. Also known as rule of false position. { 'reg-yə-lə 'fäls-ē }

**regular** [BOT] Having radial symmetry, referring to a flower. [ELECTROMAG] In a definite direction; not diffused or scattered, when applied to reflection, refraction, or transmission. { 'reg-yə-lər }

**regular Baire measure** [MATH] A Baire measure such that

the measure of any Baire set  $E$  is equal to both the greatest lower bound of measures of open Baire sets containing  $E$ , and to the least upper bound of closed, compact sets contained in  $E$ . { 'reg-yə-lər 'bä,mez-ər }

**regular Banach space** See reflexive Banach space. { 'reg-yə-lər 'bä,näk ,späs }

**regular Borel measure** [MATH] A Borel measure such that the measure of any Borel set  $E$  is equal to both the greatest lower bound of measures of open Borel sets containing  $E$ , and to the least upper bound of measures of compact sets contained in  $E$ . Also known as Radon measure. { 'reg-yə-lər bō'rel ,mez-ər }

**regular connective tissue** [HISTOL] Connective tissue in which the fibers are arranged in definite patterns. { 'reg-yə-lər kə'nek-tiv 'tish-ū }

**regular cluster** [ASTRON] A galaxy cluster that shows a smooth, centrally concentrated distribution of galaxies and an overall symmetric shape. { 'reg-yə-lər 'klās-tər }

**regular curve** [MATH] A curve that has no singular points. { 'reg-yə-lər 'kərv }

**regular dodecahedron** [CRYSTAL] See pyritohedron. [MATH] A regular polyhedron of 12 faces. { 'reg-yə-lər dō,dek-ə'hē-drən }

**regular element** [IND ENG] An element that occurs with a fixed frequency in each work cycle. Also known as repetitive element. { 'reg-yə-lər 'el-ə-mənt }

**regular expression** [COMPUT SCI] A formal description of a language acceptable by a finite automaton or for the behavior of a sequential switching circuit. { 'reg-yə-lər ik'spres-ən }

**regular extension** [MATH] An extension field  $K$  of a field  $F$  such that  $F$  is algebraically closed in  $K$  and  $K$  is separable over  $F$ ; equivalently, an extension field  $K$  of a field  $F$  such that  $K$  and  $\bar{F}$  are linearly disjoint over  $F$ , where  $\bar{F}$  is the algebraic closure of  $F$ . { 'reg-yə-lər ik'sten-ən }

**regular function** [MATH] An analytic function of one or more complex variables. { 'reg-yə-lər 'fəŋk-shən }

**Regularia** [INV ZOO] An assemblage of echinoids in which the anus and periproct lie within the apical system; not considered a valid taxon. { ,reg-yə-lar-ē-ə }

**regular icosahedron** [MATH] A 20-sided regular polyhedron, having five equilateral triangles meeting at each face. { 'reg-yə-lər i,käs-ə'hē-drən }

**regularization** [QUANT MECH] A formal procedure used to eliminate ambiguities which arise in evaluating certain integrals in a quantized field theory; corresponds to adding extra fields whose masses are allowed to approach infinity. { ,reg-yə-lər ə'zā-shən }

**regular lay** [DES ENG] The lay of a wire rope in which the wires in the strand are twisted in directions opposite to the direction of the strands. { 'reg-yə-lər 'lä }

**regular-lay left twist** See left-laid. { 'reg-yə-lər 'lä 'left 'twist }

**regular map** See normal map. { 'reg-yə-lər 'map }

**regular motor oil** [MATER] A petroleum lubricating oil suitable for use in internal combustion engines under normal operating conditions. { 'reg-yə-lər 'mōd-ər ,oil }

**regular octahedron** [MATH] A regular polyhedron of eight faces. { 'reg-yə-lər ,äk-tə'hē-drən }

**regular permutation group** [MATH] A permutation group of order  $n$  on  $n$  objects, where  $n$  is a positive integer. { 'reg-yə-lər ,pərm-yə'tā-shən ,grüp }

**regular polygon** [MATH] A polygon with congruent sides and congruent interior angles. { 'reg-yə-lər 'päl-i,gän }

**regular polyhedron** [MATH] A polyhedron all of whose faces are regular polygons, and whose polyhedral angles are congruent. { 'reg-yə-lər ,päl-i'hē-drən }

**regular polymer** [CHEM] A polymer whose molecules possess only one kind of constitutional unit in a single sequential structure. { 'reg-yə-lər 'päl-ə-mər }

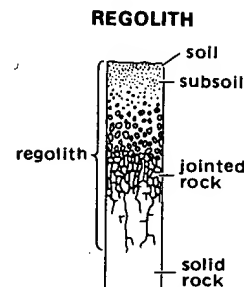
**regular prism** [MATH] A right prism whose bases are regular polygons. { 'reg-yə-lər 'priz-əm }

**regular reflection** See specular reflection. { 'reg-yə-lər ri'flek-shən }

**regular reflector** See specular reflector. { 'reg-yə-lər ri'flek-tər }

**regular representation** [MATH] A regular representation of a finite group is an isomorphism of it with a group of permutations. { 'reg-yə-lər ,repr-ə-zən'tā-shən }

**regular sampling** [MIN ENG] The continuous or intermittent sampling of the same coal or coke received regularly at a given point. { 'reg-yə-lər 'sāmpliŋ }



Cross section through the regolith showing the components.

# REGULAR LAY



Drawing of wire rope wound in regular lay showing position of the wires and strands.

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Periodic table of the chemical elements showing the position of nickel.

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